Chemical Download Help

This is an archive of all chemicals in the ClinPGx knowledgebase. Not all of these chemicals have been involved in ClinPGx annotations.

Multiple "Type" values can be assigned to a given entry since the same substance can be used in different contexts. The "Type" values used for Drugs & Chemicals are as follows:

- Drug = A chemical substance used in the treatment, cure,prevention, or diagnosis of disease.
- Metabolite = Any intermediate or product resulting from metabolism.
- Ion = An atomic or molecular particle having a net electric charge.
- Drug Class = A drug class is a group of medications that may work in the same way, have a similar chemical structure, or are used to treat the same health condition.
- Biological Intermediate = An endogenous small molucule or ion.
- Small Molecule = An electrically neutral entity consisting of more than one atom.
- Prodrug = A compound that must undergo chemical conversion by metabolic processes before becoming the pharmacologically active drug for which it is a prodrug.

Columns in this archive:

1. ClinPGx Accession Id = Identifier assigned to this chemical by ClinPGx
2. Name = Name ClinPGx uses for this chemical
3. Generic Names = Known generic names for this chemical, comma-separated and "-enclosed
4. Trade Names = Known trade names for this chemical, comma-separated and "-enclosed
5. Brand Mixtures = Known brand mixtures this chemical is in, comma-separated and "-enclosed
6. Type = Categories ClinPGx has assigned to this chemical, can be more than one, possible values: Drug, Metabolite, Ion, Drug Class, Biological Intermediate, Small Molecule, Prodrug
7. Cross-references = References to other resources in the form "resource:id", comma-separated
8. SMILES = The SMILES structure for this chemical
9. InChI = The InCHI key for this chemical
10. Dosing Guideline = "Yes" if ClinPGx has annotated a guideline with this chemical, "No" otherwise
11. External Vocabulary = Term for this chemical in another vocabulary in the form "vocabulary:id", comma-separated
12. Clinical Annotation Count = The number of clinical annotations referencing this chemical
13. Variant Annotation Count = The number of variant annotations referencing this chemical
14. Pathway Count = the number of pathways referencing this chemical
15. VIP Count = The number of VIPs referencing this chemical
16. Dosing Guideline Sources = The data sources that have guidelines about this chemical (and "no recommendation" if that source has no recommendations for this chemical)
17. Top Clinical Annotation Level = The top level of ClinPGx clinical annotation about this chemical
18. Top FDA Label Testing Level = The top PGx Testing Level from the FDA about this chemical
19. Top Any Drug Label Testing Level = The top PGx Testing Level from any label source about this chemical
20. Label Has Dosing Info = Does any label annotaton have information about dosing information for this chemical
21. Has Rx Annotation = Does this chemical have an Rx Annotation
22. RxNorm Identifiers = the RxNorm IDs for this chemical
    ATC Identifiers = the ATC IDs for this chemical

23.
24. PubChem Compound Identifiers = the PubChem Compound IDs for this chemical
25. Top CPIC Pairs Level = The top CPIC gene-drug pair level for this drug
26. FDA Label has Prescribing Info = "Yes" if there is an annotated FDA drug label with a Prescribing info section, "No" otherwise
27. In FDA PGx Association Sections = The sections of the FDA Table of Pharmacogenetic Associations that this chemical appears in